



Substance

Beilstein Registry Number	3125876
CAS Registry Number	133448-54-1, 148917-32-2
Chemical Name	butyl- <i>trans</i> -cinnamyl sulfide
Autoname	(3-butylsulfanyl-propenyl)-benzene
Molecular Formula	C ₁₃ H ₁₈ S
Molecular Weight	206.35
Lawson Number	5345, 319
Structure Keyword	Stereo compound
Compound Type	isocyclic
Constitution ID	2288675
Tautomer ID	2986537
Beilstein Reference	4-06-00-03805, 6-06
Entry Date	1990/02/15
Update Date	1994/02/18

Reaction 1 of 7

Reaction ID	<u>416096</u>
Reactant BRN	3125876 butyl- <i>trans</i> -cinnamyl sulfide
Product BRN	<u>3129601</u> (+)-butyl- <i>trans</i> -cinnamyl sulfoxide
No. of Reaction Details	2
Reaction Classification	Preparation
Reagent	aqueous H ₂ O ₂ acetone

Note 1 Handbook

Ref. 1 1627251; Journal; Barnard; Hargrave; ACACAM; Anal.Chim.Acta; 5; 1951; 536, 544;

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Reaction ID	<u>3745298</u>
Reactant BRN	<u>741973</u> 3 <i>t</i> -phenyl-prop-2-en-1-ol <u>1730908</u> butane-1-thiol
Product BRN	3125876 butyl- <i>trans</i> -cinnamyl sulfide
No. of Reaction Details	1
Reaction Classification	Preparation
Yield	89 percent (BRN=3125876)
Catalyst	BF ₃ *Et ₂ O

Solvent	CH ₂ Cl ₂
Time	43 hour(s)
Other Conditions	Ambient temperature
Ref. 1	<u>5717632</u> ; Journal; Tsay, Shwu-Chen; Lin, Lung Ching; Furth, Paul A.; Shum, Chi C.; King, Daniel B.; et al.; SYNTBF; Synthesis; EN; 3; 1993; 329-334;

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Reaction ID	<u>7952337</u>
Reactant BRN	3125876 butyl- <i>trans</i> -cinnamyl sulfide
No. of Reaction Details	1
Reaction Classification	Chemical behaviour (half reaction)
Temperature	75 C
Other Conditions	Autoxidation
Subject Studied	Kinetics
Note 1	Handbook
Ref. 1	<u>1415668</u> ; Journal; Bateman; Cunneen; JCSOA9; J.Chem.Soc.; 1955; 1596;

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Reaction ID	<u>7967051</u>
Reactant BRN	<u>605970</u> benzene-1,4-diol 3125876 butyl- <i>trans</i> -cinnamyl sulfide
No. of Reaction Details	1
Reaction Classification	Chemical behaviour (half reaction)
Temperature	75 C
Other Conditions	Autoxidation
Subject Studied	Kinetics
Note 1	Handbook
Ref. 1	<u>1415668</u> ; Journal; Bateman; Cunneen; JCSOA9; J.Chem.Soc.; 1955; 1596;

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Reaction ID	<u>7968349</u>
Reactant BRN	<u>984320</u> dibenzoyl peroxide 3125876 butyl- <i>trans</i> -cinnamyl sulfide
No. of Reaction Details	1
Reaction Classification	Chemical behaviour (half reaction)
Temperature	75 C
Other Conditions	Autoxidation
Subject Studied	Kinetics
Note 1	Handbook